

(FILE 'HOME' ENTERED AT 13:01:13 ON 03 MAR 2004)

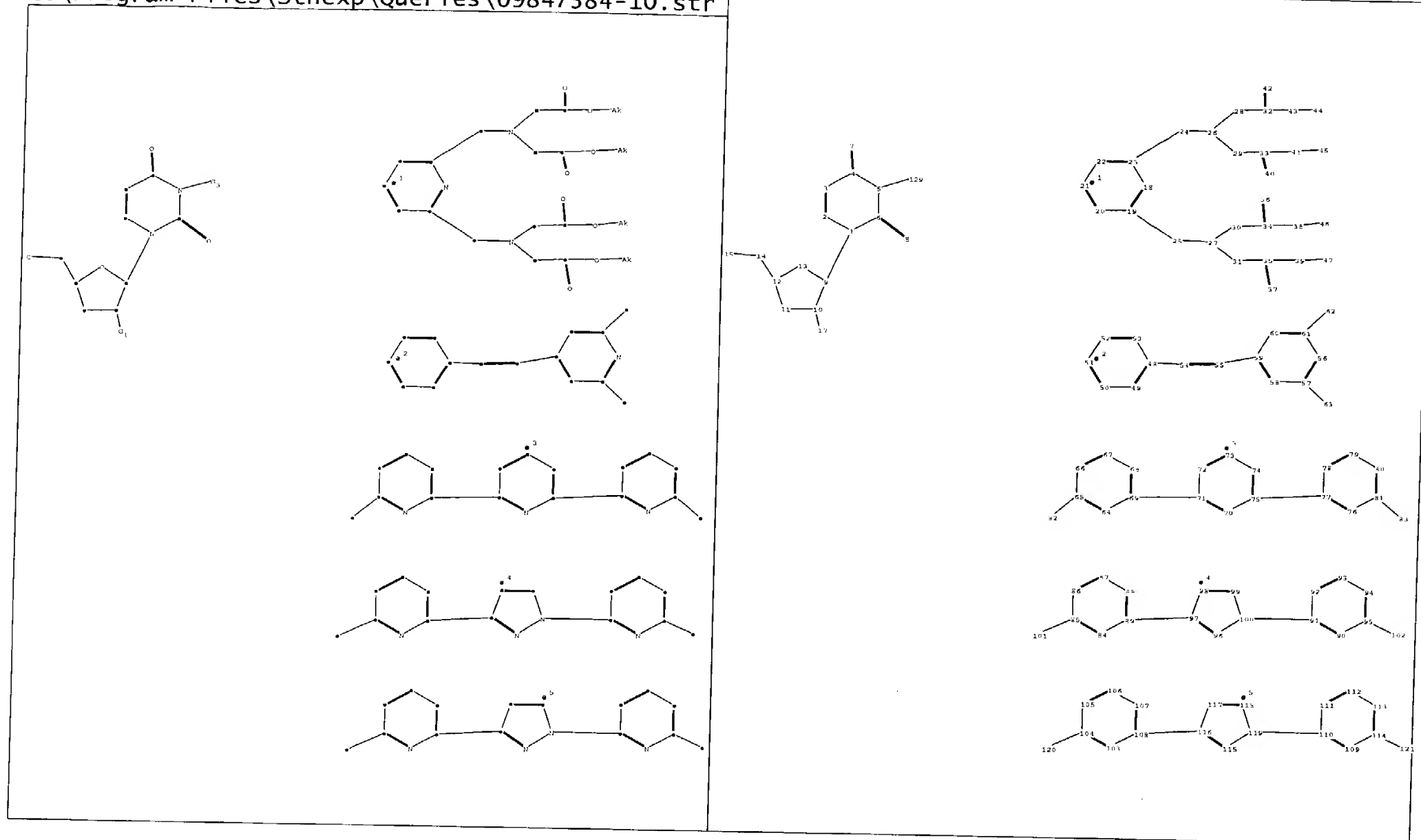
FILE 'REGISTRY' ENTERED AT 13:01:30 ON 03 MAR 2004

L1               STRUCTURE UPLOADED

L2               0 S L1 SSS SAM

L3               0 S L1 SSS FULL

=>



chain nodes :

7 8 14 15 17 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41  
 42 43 44 45 46 47 54 55 62 63 82 83 101 102 120 121 129

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 18 19 20 21 22 23 48 49 50 51 52 53 56  
 57 58 59 60 61 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80  
 81 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 103 104 105  
 106 107 108 109 110 111 112 113 114 115 116 117 118 119

chain bonds :

1-9 4-7 5-129 6-8 10-17 12-14 14-15 19-25 23-24 24-26 25-27 26-28 26-29  
 27-30 27-31 28-32 29-33 30-34 31-35 32-42 32-43 33-40 33-41 34-36 34-38 35-37  
 35-39 38-46 39-47 41-45 43-44 48-54 54-55 55-59 57-63 61-62 65-82 69-71 75-77  
 81-83 85-101 89-97 91-100 95-102 104-120 108-116 110-119 114-121

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 18-19 18-23 19-20 20-21  
 21-22 22-23 48-49 48-53 49-50 50-51 51-52 52-53 56-57 56-61 57-58 58-59 59-60  
 60-61 64-65 64-69 65-66 66-67 67-68 68-69 70-71 70-75 71-72 72-73 73-74 74-75  
 76-77 76-81 77-78 78-79 79-80 80-81 84-85 84-89 85-86 86-87 87-88 88-89 90-91  
 90-95 91-92 92-93 93-94 94-95 96-97 96-100 97-98 98-99 99-100 103-104 103-108  
 104-105 105-106 106-107 107-108 109-110 109-114 110-111 111-112 112-113 113-114  
 115-116 115-119 116-117 117-118 118-119

exact/norm bonds :

1-2 1-6 1-9 2-3 3-4 4-5 4-7 5-6 5-129 6-8 9-10 9-13 10-11 10-17 11-12  
 12-13 14-15 24-26 25-27 26-28 26-29 27-30 27-31 32-42 32-43 33-40 33-41 34-36  
 34-38 35-37 35-39 38-46 39-47 41-45 43-44 91-100 96-97 96-100 97-98 98-99  
 99-100 110-119 115-116 115-119 116-117 117-118 118-119

exact bonds :

12-14 19-25 23-24 28-32 29-33 30-34 31-35 48-54 54-55 55-59 57-63 61-62 65-82  
 69-71 75-77 81-83 85-101 89-97 95-102 104-120 108-116 114-121

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23 48-49 48-53 49-50 50-51 51-52 52-53 56-57  
 56-61 57-58 58-59 59-60 60-61 64-65 64-69 65-66 66-67 67-68 68-69 70-71 70-75  
 71-72 72-73 73-74 74-75 76-77 76-81 77-78 78-79 79-80 80-81 84-85 84-89 85-86  
 86-87 87-88 88-89 90-91 90-95 91-92 92-93 93-94 94-95 103-104 103-108 104-105  
 105-106

106-107 107-108 109-110 109-114 110-111 111-112 112-113 113-114

G1:H,O,S,N

G2:[\*1],[\*2],[\*3],[\*4],[\*5]

G3:C,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom  
21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS  
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS  
39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS  
48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:CLASS 55:CLASS 56:Atom  
57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:CLASS 63:CLASS 64:Atom 65:Atom  
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom  
76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:CLASS 83:CLASS 84:Atom  
85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom  
95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 101:CLASS 102:CLASS 103:Atom  
104:Atom 105:Atom 106:Atom 107:Atom 108:Atom 109:Atom 110:Atom 111:Atom 112:Atom  
113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:CLASS  
121:CLASS 129:CLASS